

Effect of Anharmonicity of Interatomic Potential on Strain Distribution in Semiconductor Nanostructures

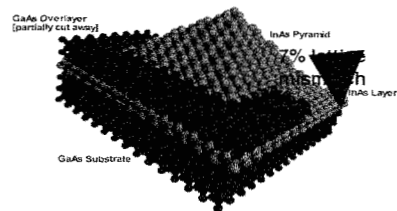
Olga L. Lazarenkova¹ (LOL@jpl.nasa.gov),

Paul von Allmen¹, Fabiano Oyafuso¹, Seungwon Lee¹, and Gerhard Klimeck^{1,2}

¹ – Jet Propulsion Laboratory, California Institute of Technology MS: 169-315, 4800 Oak Grove Dr., Pasadena CA 91109-8099

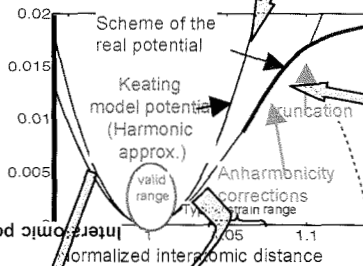
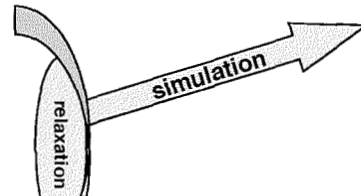
² - School of Electrical Engineering, Purdue University, West Lafayette, IN 47906

Large lattice mismatch in semiconductor nanostructures



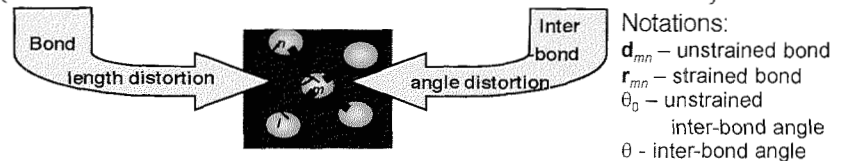
Large built-in strain affects most of the QD properties

Parameters of the Simulated InAs/GaAs QD structure:
 • Dome QD: base 8 nm, height 3.5 nm
 • Width of the wetting layer 1nm
 • Periodicity: lateral 17 nm, along growth direction 8.5 nm



Usually used – Keating's Valence Force Field Model (VFFM)

$$E = \frac{3}{8} \sum_{atoms} \left\{ \sum_{Neighbors} \frac{\alpha_{mn}}{d_{mn}^2} (\mathbf{r}_{mn} \cdot \mathbf{r}_{mn} - d_{mn} \cdot d_{mn})^2 + \sum_{couples} \frac{\sqrt{\beta_{mn}\beta_{ml}}}{d_{mn}d_{ml}} (\mathbf{r}_{mn} \cdot \mathbf{r}_{ml} - d_{mn} \cdot d_{ml})^2 \right\}$$

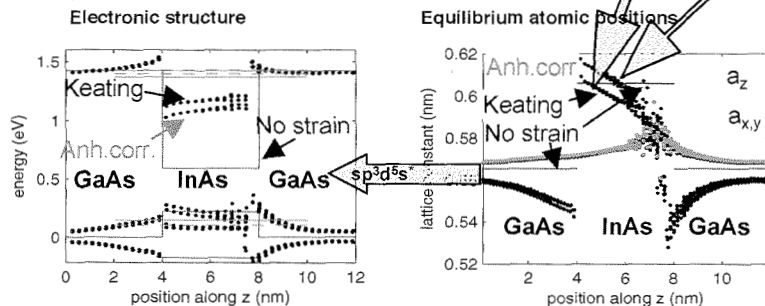


Anharmonicity corrections to VFF parameters:

$$\alpha = \alpha_0 \left[1 - A \frac{(r_{mn}^2 - d_{mn}^2)}{d_{mn}^2} \right]$$

$$\beta = \beta_0 \times \left[1 - C \frac{r_{mn}r_{ml} - d_{mn}d_{ml}}{d_{mn}d_{ml}} \right] \times [1 - B(\cos\theta - \cos\theta_0)]$$

A, B, and C were obtained by fitting the experimental phonon spectra of strained materials



Material	α_0 (N/m)	β_0 (N/m)	A	B	C
Si	48.5	13.8	7.67	4.67	4.53
Ge	38.0	12.0	8.33	4.80	5.08
GaAs	41.49	8.94	7.20	7.62	6.40
InAs	35.18	5.49	7.61	4.78	6.45
GaSb	33.16	7.22	7.96	6.54	6.07
InSb	29.61	4.77	7.53	9.62	6.46
AlSb	35.35	6.77	8.28	7.58	7.17

Conclusions

- Built-in strain strongly affects the electronic structure of nanostructures
- Anharmonicity in valence-force-field results in a strain distribution leading to a 100 meV improvement of computed (within tight binding $sp^3d^5s^*$) band offsets compared to experiment



Acknowledgements:

- National Research Associateship Award at Jet Propulsion Laboratory for O.L.L.
- Grants from ARDA, ONR, JPL, NASA, and NSF (Grant No. EEC-0228390)



Please, put your comments and coordinates HERE

